(E)-2-Octene, 4-methyl

Inchi: InChI=1S/C9H18/c1-4-6-8-9(3)7-5-2/h5,7,9H,4,6,8H2,1-3H3/b7-5+
InchiKey: HJJLGGXQXVNFBB-FNORWQNLSA-N
Formula: C9H18
SMILES: CC=CC(C)CCCC
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
gf	102.68	kJ/mol	Joback Method
hf	-117.15	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	35.20	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	857.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	860.00		NIST Webbook
tb	409.04	K	Joback Method
tc	584.08	K	Joback Method
tf	171.11	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.03	J/mol×K	409.04	Joback Method
cpg	272.42	J/mol×K	438.21	Joback Method
cpg	286.19	J/mol×K	467.39	Joback Method
cpg	299.36	J/mol×K	496.56	Joback Method
cpg	311.95	J/mol×K	525.73	Joback Method
cpg	323.98	J/mol×K	554.90	Joback Method

cpg	335.48	J/mol×K	584.08	Joback Method
dvisc	0.0104021	Pa×s	171.11	Joback Method
dvisc	0.0028673	Pa×s	210.77	Joback Method
dvisc	0.0011887	Pa×s	250.42	Joback Method
dvisc	0.0006269	Pa×s	290.07	Joback Method
dvisc	0.0003857	Pa×s	329.73	Joback Method
dvisc	0.0002633	Pa×s	369.38	Joback Method
dvisc	0.0001936	Pa×s	409.04	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R42643&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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